

ELECTRONIC CONTRIBUTION TO THE THERMAL DIFFUSIVITY: $\text{DyBa}_2\text{Cu}_3\text{O}_{7-y}$ AND $\text{Y}_{0.9}\text{Ca}_{0.1}\text{Ba}_2\text{Cu}_3\text{O}_{7-z}$

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Received 20 February 1998

Revised 6 April 1998

The electronic contribution to the specific heat and the thermal conductivity of high- T_c superconductors is calculated with a three-dimensional band structure including saddle points and a Lawrence-Doniach coupling between the CuO_2 planes. The electronic thermal diffusivity is deduced for s - and d -wave symmetry of the order parameter. Data on $\text{DyBa}_2\text{Cu}_3\text{O}_{7-y}$ and $\text{Y}_{0.9}\text{Ca}_{0.1}\text{Ba}_2\text{Cu}_3\text{O}_{7-z}$ and theory are in good agreement on the change of the slope near T_c .

1. Introduction

The thermal diffusivity α_{tot} arises as a coefficient in the heat balance equation,¹ as the ratio between the thermal conductivity κ_{tot} and the product of the specific heat C_{tot} and the density ρ . Since κ_{tot} and C_{tot} can be decomposed into an electronic (index e) and a phonon (index ph) contribution, one has

$$\alpha_{\text{tot}} = \frac{\kappa_e + \kappa_{\text{ph}}}{(C_e + C_{\text{ph}})\rho} = \frac{\kappa_e}{\rho(C_{\text{ph}} + C_e)} + \frac{\kappa_{\text{ph}}}{\rho(C_{\text{ph}} + C_e)} = \alpha_e + \alpha_{\text{ph}} \quad (1)$$

defining as such the electronic thermal diffusivity α_e .

From a microscopic point of view, the diffusivity can be related to the mean free path l of the heat carriers¹ and their velocity v : $\alpha_{\text{tot}} = vl/3$.

The presence of van Hove singularities in the density of states near the Fermi level are taken into account in calculation of α_e , C_e and κ_e for comparison to our experimental data. The effects of those singularities are observed on the superconductivity state and on the normal state, e.g. on the pseudogap of overdoped compounds. Moreover, a large number of experiments favors a d -wave gap symmetry over the s -wave case in the *hole-doped* cuprate compounds.

2. Theoretical Model

The electronic specific heat C_e of a superconductor can be calculated² for a quasi-particle energy spectrum $E(\mathbf{k}) = \sqrt{(\epsilon(\mathbf{k}) - \epsilon_F)^2 + \Delta(\mathbf{k})^2}$ where $\epsilon(\mathbf{k})$ is the band

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structure near the Fermi energy ϵ_F

$$\epsilon(\mathbf{k}) - \epsilon_F = \frac{\hbar^2}{2m^*} (k_x^2 + k_y^2) + J \cos(k_z d) \quad (2)$$

and

$$\epsilon(\mathbf{k}) - \epsilon_F = \frac{\hbar^2}{2m^*} k_x k_y \quad (3)$$

where m^* is the effective mass of electrons in the ab (CuO_2) plane, J and d are respectively the coupling energy and the distance between CuO_2 planes. J values are small (< 10 meV) for two-dimensional systems and large (≈ 30 meV) for three-dimensional compounds. $\Delta(\mathbf{k})$ is the k -dependent (constant) energy gap in the d -wave (s -wave) case.³ The phonon contribution C_{ph} can be calculated using the Debye model.¹ The electronic thermal conductivity can be calculated by a variational method⁴ considering scattering of electrons by point defects and acoustic phonons.

3. Theoretical Results

For illustration, we have fixed different *common* values of the physical parameters corresponding to a virtual $\text{YBa}_2\text{Cu}_3\text{O}_7$, namely an energy gap $\Delta = 20$ meV, an effective mass $m_{xy} = 8m_e$, a critical temperature $T_c = 90$ K, a Debye temperature $\theta = 350$ K and an arbitrary density $\rho = 6.0$ g/cm³.

In Fig. 1, the normalized electronic thermal diffusivity $\alpha_{e,n} = \alpha_e(T)/\alpha_e(T_c)$ is plotted versus temperature in the s -wave case combined with the band structure Eq. (2) and in the d -wave case with the band structure Eq. (3) after calculation of κ_e , C_e and C_{ph} . The normal state is characterized by a T^{-1} behavior. A discontinuity is found in both cases at the critical temperature. The electronic diffusivity jump

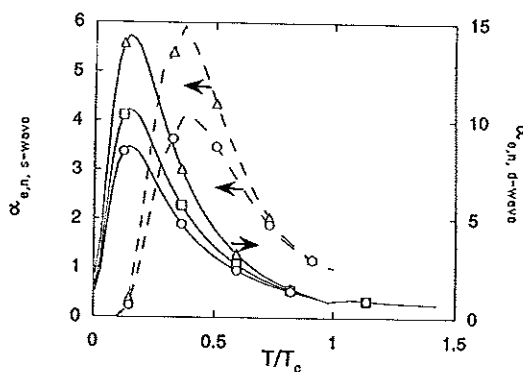


Fig. 1. Normalized electronic contribution to the thermal diffusivity calculated in the s -wave (broken lines) and d -wave cases (solid lines). The triangles, squares and circles correspond to $N = 0.05, 0.075$ and 0.1 .

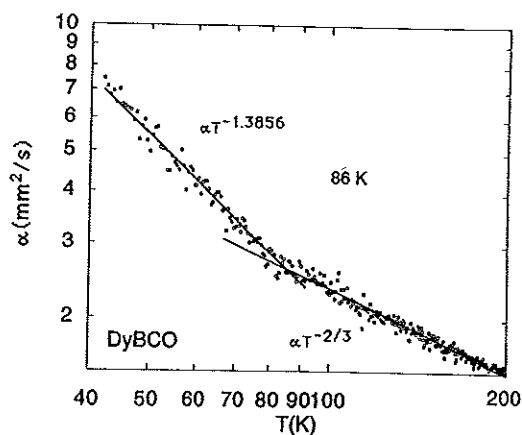
(2)

(3)

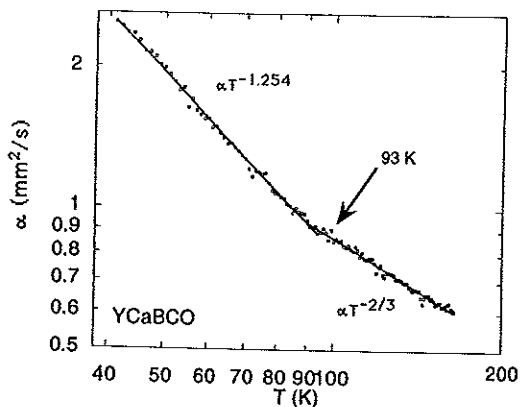
plane, J and d are O_2 planes. J value (≈ 30 meV) for (at) energy gap in calculated using calculated by a vari- effects and acoustic

physical parameters $\Delta = 20$ meV, an T_c by temperature

$\alpha_e(T)/\alpha_e(T_c)$ is e band structure calculation of κ_e , A discontinuity diffusivity jump



(a)



(b)

Fig. 2. Thermal diffusivity of (a) $\text{DyBa}_2\text{Cu}_3\text{O}_{7-y}$ sample and (b) $\text{Y}_{0.9}\text{Ca}_{0.1}\text{Ba}_2\text{Cu}_3\text{O}_{7-y}$ sample.

is about 20% in d -wave case and 5% in the s -wave case. This can be explained by the presence of the van Hove singularity in the electronic density of states in the d -wave case. The diffusivity behaves like $T^{-\sigma}$ ($\sigma \in [1.7, 2.4]$) and presents a maximum below T_c . At very low temperature, the electronic thermal diffusivity behaves like an exponential in the s -wave case and as a power law in the d -wave case.

The thermal diffusivity of a $\text{DyBa}_2\text{Cu}_3\text{O}_{7-y}$ and of a $\text{Y}_{0.9}\text{Ca}_{0.1}\text{Ba}_2\text{Cu}_3\text{O}_{7-z}$ sample was measured using the matrix method⁵ (Fig. 2(a)-(b)). A change in slope is found at T_c as expected. A $T^{-2/3}$ behavior is found above T_c and in the superconducting state, $\sigma = 1.25$ and 1.39 values are found respectively.

ated in the s -wave cases correspond to

Acknowledgments

Part of this work has been financially supported by the ARC 94-99/174 contract. S. Dorbolo benefits from a FRIA research fellowship. Thanks to Prof. H. W. Vanderschueren for allowing us to use the MIEL Laboratory and to Prof. R. Cloots and Prof. I. Nedkov for the synthesis of the samples.

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